Available online at www.sciencedirect.com
SciVerse ScienceDirect
Procedia - Social and Behavioral Sciences 53 (2012) 399 – 409
Procedia
Social and Behavioral Sciences

SIIV - 5th International Congress - Sustainability of Road Infrastructures

Discrete Element Modelling of Influences of Grain Shape and Angularity on Performance of Granular Mixes for Asphalts

Giulio Dondi [a], Andrea Simone [a], Valeria Vignali [a,*], Giulia Manganelli [a]

[a] *University of Bologna, DICAM Department, Viale Risorgimento2, 40136, Bologna, Italy*

Abstract

The greater part of asphalt mixtures is composed of aggregates. This means that particular features, such as shape and angularity, are the primary factors that affect the development of the mechanical performance of asphalt pavements. In order to investigate the combined effect of grain shape and angularity on the packing and stability of an aggregate's assembly for asphalt mixes, the authors have performed an experimental program using 3D Discrete Element Method. The results obtained from triaxial tests and from statistical analysis of the distribution of particle-particle contact forces show that the grain shape and angularity significantly affect the assembly behaviour.

Keywords: Discrete element modelling; triaxial test; aggregate shape; particle interaction; asphalt

1. Introduction

The properties of aggregates used in hot-mix asphalt (HMA) have a significant influence on the engineering properties of the pavement in which they are used. The shape and angularity of particles, in fact, influence their mutual interactions and are related to durability, workability, shear resistance, tensile strength and fatigue response of the pavement layer. So it becomes important to evaluate the characteristics of the grains very carefully.

The role of the aggregate's shape and angularity in controlling the performance of asphalt mixtures has been highlighted by many researchers. Campen and Smith (1948) found that, when crushed aggregates were used instead of rounded ones, the stability of HMA mixtures increased from 30 to 90% [1]. Ishai and Gellber (1982) evaluated different asphalt mixtures containing four aggregates types and they showed that there was a significant increase in stability with an increase in the geometric irregularities of the particles [2]. Sanders and Dukatz (1992)

* Corresponding author. Tel.: +39 051 2093522; fax: +39 051 2093527.
E-mail address: valeria.vignali@unibo.it

 doi:10.1016/j.sbspro.2012.09.891

reported on the influence of coarse aggregate angularity on permanent deformation of four interstate sections of HMA pavements in Indiana [3]. One of the four sections developed permanent rutting within two years of service. They found that mixtures used in the binder course and the surface course of the rutted section had lower amounts of angular coarse aggregate compared to the other three sections. Kandhal and Parker (1998) pointed out that presence of excessive flat and elongated aggregate particles is undesirable in HMA mixtures because they tend to break down during production and construction, thus affecting mix durability [4]. Cheung and Dawson (2002) concluded that roundness and angularity are the main factors affecting the ultimate shear strength and permanent deformation. It was therefore clearly established that increasing the particles' angularity improves grains interlocking and packing and, as a result, the fatigue performance of the asphalt mixture [5].

In reality, it is very difficult to measure and quantify the degree of aggregate interlocking directly, because the fundamental theories of packing for particles are still not entirely clear and most of the existing methods are confined to two dimensional assemblies or have difficulties in distinguishing between contacts and near-contacts [6]. Because Discrete Particle Elements Method (DEM) considers particles as distinct interacting bodies, it is an excellent tool to investigate the micro-mechanical behavior of granular assemblies. Interactions between particles are considered to be a dynamic process with states of equilibrium developing whenever the internal forces are in balance. Contact forces and displacements of a stressed assembly are found by tracing the movements of individual particles. The calculations in the DEM procedure involve first applying Newton's second law to the particles and then a force-displacement law to the points where the particles make contact [7].

Many researchers have investigated the effect of aggregate characteristics on the behavior of asphalt mixtures, using the discrete element modeling approach. Buttlar and You (2001) simulated by DEM the behavior of asphalt mixture in indirect tension testing and they highlighted the significant contribution of aggregate's interaction, suggesting the need to utilize realistic aggregate shapes in micro-structure models [8]. Dondi et al. (2007) presented a DEM model to simulate the fatigue performance of an asphalt pavement, modeled by clumps with different shapes [9]. The results showed that the introduction of parameters, such as the shape and angularity of aggregates, greatly influenced the system's response and, in particular, it helped in detecting new starting points of cracks. Mahmoud et al. (2010) introduced an approach that combined the discrete element method with image processing techniques in order to analyze the combined effects of aggregate gradation, shape, stiffness and strength on hot-mix asphalt's resistance to fracture [10]. The results showed that the required aggregate strength depends strongly upon the aggregate's characteristics. Shen and Yu (2011) have studied aggregate packing, which, as it affects the way aggregate particles form a skeleton to transmit and distribute traffic loads, influences the stability and mechanical performance of the mix [6]. They have developed a two-step procedure, using a discrete element modeling simulation method: the first one involved evaluating the effect of size distribution, while the second investigated the combined effect of size distribution and shape impact. The study demonstrated that aggregate size distribution plays a significant role, affecting both the volumetric and contact characteristics of a packed structure, such as an asphalt mixture.

A commercially available three-dimensional DEM code called Particle Flow Code (PFC), developed by Itasca Consulting Group, was used in this study [11]. In PFC3D, particles are spheres (balls) that move independently of each other and only interact at the contact points. One of the main advantages of a DEM simulation in PFC3D is that it can easily carry out a thorough inspection of the spheres' contacts inside the model, something that is difficult to observe in the field or laboratory.

2. The experimental program

An experimental program was developed to understand how the packing characteristics of aggregate particles in granular mixes for asphalt can be affected by the shape and interlocking of grains [12].

An ideal granular material, stainless steel spheres, was used in this research [Fig. 1].

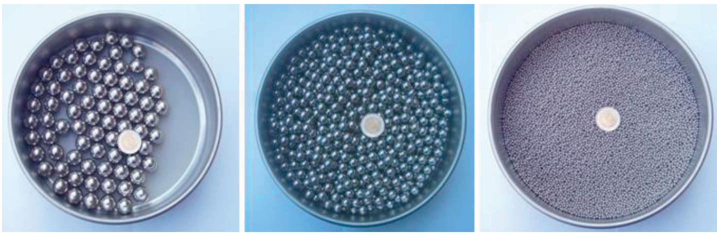


Fig. 1. steel spheres used in the research (diameter of 18, 11 and 2.77 mm)

There are obviously differences between steel spheres and the real aggregates in asphalt mixtures; however, by comparing DEM simulations with laboratory tests carried out on this "ideal material", it is possible to replicate the geometry of the DEM model accurately [Fig. 2]. For the steel spheres were selected a density of 7,800 kg/m^3 and the gradation shown in Table 1.

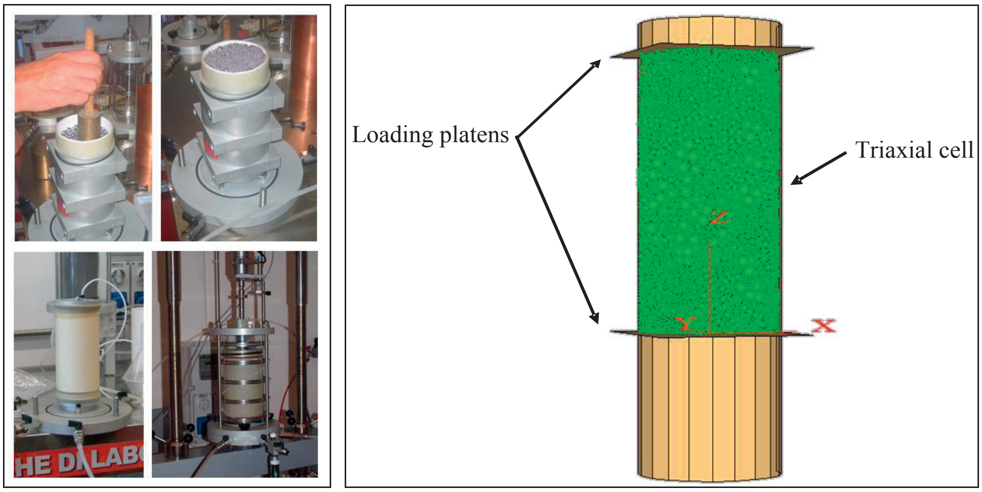


Fig. 2. (a) laboratory triaxial test; (b) DEM model

Table 1. Gradation of steel spheres

Sieve size [mm]	19	12.5	9.5	4.75	2.36	1.18	0.6	0.3	0.15	0.075
% Passing	100	76.5	35.3	35.3	0	0	0	0	0	0

Two specimen types were considered:

- one uniform, containing spheres;
- one non-uniform, containing a mixture of spheres and angular grains formed of spheres.

The first mixture (1S), according to gradation shown in Table 1, was composed of 32,886 spheres. The other assemblies, consisting of spheres and angular grains, according to gradation of Table 1, were formed of:

- 32,204 spheres, with a diameter of 2.77 mm, as the first mixture 1S;
- angular grains that replace the medium and large spheres of the mixture 1S.

Three types of angular grains were chosen, formed of two (2C), three (3C) or four spheres (4C).

So that there could be a good comparison between the four series of grains, the angular particles and the spheres have the same external diameter and the same total particle volume, for each size range within the gradation curve [Fig. 3, Table 2].

Figure 4 shows an example of angular grain formed of three spheres, obtained by sticking together the steel spheres using a cold-weld compound.

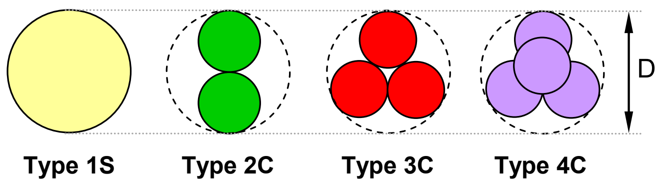


Fig. 3. types of mix of spheres and angular grains

Table 2. Number and diameter of particles of the examined mixtures

Mix type	Mix elements	Particle sieve size interval [mm]				
		0.075 - 2.36	2.36 - 4.75	4.75 - 9.5	9.5 - 12.5	12.5 - 19
1S	Spheres number	-	32,204	-	605	77
	Spheres diameter [mm]	-	2.77	-	11	18
2C	Spheres number	-	32,204	-	-	-
	Spheres diameter [mm]	-	2.77	-	-	-
	Angular grains number	-	-	-	2,423	308
	Angular grains diameter [mm]	-	-	-	11	18
3C	Spheres number	-	32,204	-	-	-
	Spheres diameter [mm]	-	2.77	-	-	-
	Angular grains number	-	-	-	1,615	205
	Angular grains diameter [mm]	-	-	-	11	18
4C	Spheres number	-	32,204	-	-	-
	Spheres diameter [mm]	-	2.77	-	-	-
	Angular grains number	-	-	-	1,211	154
	Angular grains diameter [mm]	-	-	-	11	18

Fig. 4. angular grain formed of three spheres (diameter of 11 mm)

All mixes were subjected to triaxial testing. The cylindrical specimens were 100 mm in diameter and 200 mm high. All tests were strain-controlled, with the strain rate set to 1 mm/min and the confining pressure maintained constant. In particular it was set to 400 kPa and 500 kPa [Table 3].

Table 3. Confining pressure and code for examined tests

Type of mixture	1S	1S	2C	2C	3C	3C	4C	4C
Confining pressure [kPa]	400	500	400	500	400	500	400	500
Test code	1S_400	1S_500	2C_400	2C_500	3C_400	3C_500	4C_400	4C_500

For the DEM simulations, since steel spheres are an unbound material, bond models were avoided [13]. The system's behaviour was described using only a contact-stiffness model and a slip-separation model, with normal and shear stiffness set to 10^7 N/m. The aggregate-to-aggregate contact friction coefficient and the particle-boundary friction coefficient were set to 0.42 and 0 respectively. The first, in particular, was measured by the steel spheres manufacturer; the second, instead, was set to 0, according to the findings of O'Sullivan et al. (2004) [14], who performed triaxial laboratory test simulations on steel assemblies and observed no variation in the specimens' response for various particle-boundary friction coefficients. Angular grains were modeled using clumps. A clump behaves like a rigid body because the particles, from which it is made, remain at a fixed distance from each other.

3. Analysis of the internal contact force distribution

The internal forces in asphalt mixtures are very important since they control stress localization and mixture fracture. In the examined mixture they were studied at two loading stages: case II was selected at the peak force, while case I represented an intermediate force equal to 50% of the peak one. Table 4 presents the normal and shear maximum contact forces within each mix, for the two different cases.

Table 4. Maximum contact forces at different loading stages [N]

	Loading stage	Confining pressure [kPa]	Type of mixture			
			1S	2C	3C	4C
Normal contact force	I	400	416	1048	1888	2561
		500	632	1686	2137	2746
	II	400	501	1158	2210	2924
		500	713	1859	2410	3124
Shear contact force	I	400	54	310	487	930
		500	89	438	652	962
	II	400	65	343	570	1062
		500	100	483	735	1094

It shows that normal and shear contact forces increase when going from round to high angular grains. For any specified confining pressure, in fact, the 4C exhibits the highest maximum internal forces among all other mixes, when compared at the same level of loading. These results could be attributed to greater interlocking and more contacts between the particles.

During the triaxial tests, moreover, the contact force network is oriented mainly vertically, whatever the shape or angularity of the grains, reflecting the vertical orientation of the axial stress. Visual interpretation of its plots from 3D simulations shows that, as straining progresses, there are a great many vertical contacts and that these transmit significantly larger forces than the horizontal contacts.

The same trend also defines the number of contacts per particle [Table 5]. In fact, when more angular grains are added to the assembly, it increases for any specified confining pressure. On the other hand, for assemblies of grains with equal angularity, the number of contacts per particle increases when the confining pressure increases.

Table 5. Number of contacts per particle

Type of mixture	1S	1S	2C	2C	3C	3C	4C	4C
Confining pressure [kPa]	400	500	400	500	400	500	400	500
Number of contacts per particle	0.47	0.50	0.55	0.57	0.63	0.68	0.74	0.80

So it is possible to confirm that adding more angular grains to the assembly means achieving more aggregate contacts and better particle interconnection. In this way a significant improvement of fatigue performance of an asphalt pavement can be obtained because according to Cocurullo et al. (2008) [15], a high percentage of air voids may reduces the fatigue life of the specimen.

Table 6 shows the relationship between the total contact force for the two loading stage examined. It increases with an increase in applied load for the different mixtures. The rate of increase, in particular, is important because it is an indication of the aggregate resistance to fracture [10]. A low rate of increase, in fact, indicates more breakage of particles, with a reduction of the mix ability to sustain applied loads and of the internal forces among aggregate particles. From the models, the 4C is a stronger mixture than the others, which is reflected in better ability to sustain traffic loads and higher rate of increase in build up of internal forces. The 1S, instead, has the smallest rate of increase, which is an indication that aggregate breakage is more probable than in other mixtures.

Table 6. Total contact forces at different loading stages [N]

Loading stage	Confining pressure [kPa]	Type of mixture			
		1S	2C	3C	4C
I	400	143742	163429	169586	172717
	500	144292	165695	171349	173419
II	400	161019	186152	198522	214302
	500	162747	190389	205632	216639
Rate of increase of stage I on stage II	400	0.12	0.14	0.17	0.24
	500	0.13	0.15	0.20	0.25

4. Statistics of the contact network

For all modelled mixtures the contact forces have been subjected to an in-depth statistical analysis, in order to obtain useful information about the contact network and its variation during the test. It controls, in fact, the strength-deformation characteristics and particle breakage of a granular mix for asphalt.

Only contact forces at the loading stage II (case II) have been considered.

Tables 7 and 8 show the univariate summary statistics for normal and shear contact forces respectively.

Table 7. Univariate summary statistics for normal contact forces

Type of mixture	1S		2C		3C		4C	
Confining pressure [kPa]	400	500	400	500	400	500	400	500
Number of contacts	15591	16401	19208	19892	21452	23002	24754	27000
Mean [N]	8,76	8,43	8,23	8,12	7,85	7,61	7,41	6,84
Median [N]	2	3	0	0	0	0	0	0
Mode [N]	1	1	0	0	0	0	0	0
Standard deviation	26	25	87	102	61	58	52	67
Variance	694	641	7537	10422	3666	3339	2737	4490
Skewness	7	11	11	14	19	18	20	25
Kurtosis	65	210	132	203	519	530	669	824
Minimum [N]	0	0	0	0	0	0	0	0
Maximum [N]	501	713	1158	1859	2210	2410	2924	3124

Table 8. Univariate summary statistics for shear contact forces

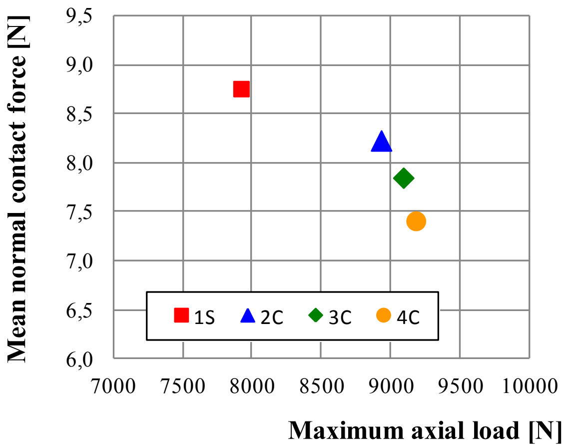
Type of mixture	1S		2C		3C		4C	
Confining pressure [kPa]	400	500	400	500	400	500	400	500
Number of contacts	15591	16401	19208	19892	21452	23002	24754	27000
Mean [N]	1,49	1,46	1,41	1,35	1,40	1,33	1,24	1,18
Median [N]	0	0	0	0	0	0	0	0
Mode [N]	0	0	0	0	0	0	0	0
Standard deviation	4	4	17	18	15	21	24	21
Variance	19	16	302	310	230	450	572	448
Skewness	6	8	13	17	25	20	29	30
Kurtosis	45	96	190	349	713	440	982	1095
Minimum [N]	0	0	0	0	0	0	0	0
Maximum [N]	65	100	343	483	570	735	1062	1094

They confirm that the degree of contact and interlocking of aggregates is a function of the shape and angularity of the grains. By adding angular grains to the assembly, in fact, the quantity and magnitude of contacts within the aggregates increase, with a better interconnection between particles for any specified confining pressure. On the other hand, for assemblies of grains with equal angularity, the number of contacts and the magnitude of contact forces increase when the confining pressure increases.

Shear contact forces are always smaller than the normal ones. For this reason in the next they have been neglected.

The mean values, moreover, show that, passing from 1S to 4C mixture, the increase of interlocking between particles leads to a more uniform distribution of internal forces, with a better interconnection between particles and a significant improvement of fatigue performance of an asphalt pavement. It achieves, in particular, a reduction of the mix "micro stiffness", because, adding angular grains to the assembly, the maximum axial load applied during the triaxial test increases and the mean normal contact force among particles decreases, for any specified confining pressure [Fig. 5].

The skewness values indicate that normal and shear contact forces distributions have a long right tail. Positive kurtosis, instead, point out that the observations cluster more and have longer tails than those in the normal distribution.



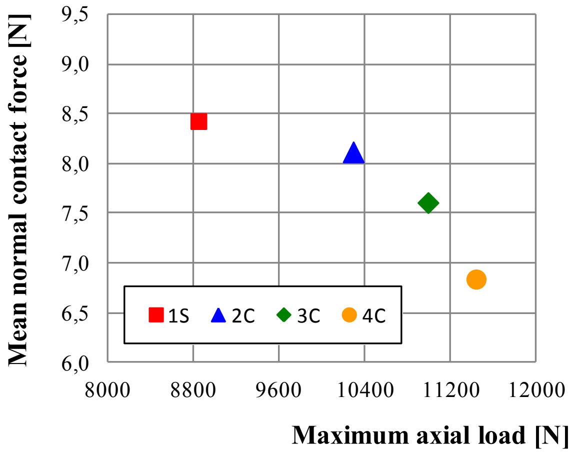


Fig. 5. (a) mean normal contact force versus maximum axial load for confining pressures of 400 kPa; (b) of 500 kPa

For all simulated test, frequency distribution of contact forces, in terms of histogram and normal probability density function, have been evaluated. Only normal contact forces at the loading stage II (case II) have been considered. Each value, in particular, has been normalized by dividing it by the mean normal contact force at that loading level.

Histograms for the examined test are similar to each other. The number of high contact forces is very small and the corresponding frequency is also very small. The mean value depend mainly on the smaller contact forces, because they are much more numerous than the large ones. The specimens, therefore, are subjected to a numerous small contact forces and a few peaks [Fig. 6].

The same trend is confirmed by the 95th percentile of the distribution, which is the value below which 95% of the observations fall, which, for assemblies of grains with equal angularity, increases when the confining pressure increases [Table 9]. On the other hand, for any specified confining pressure, when going from round to high angular grains, it decreases. It means that inside the granular mix the distribution of internal forces is more uniform with a greatly improvement of its fatigue and rutting resistance.

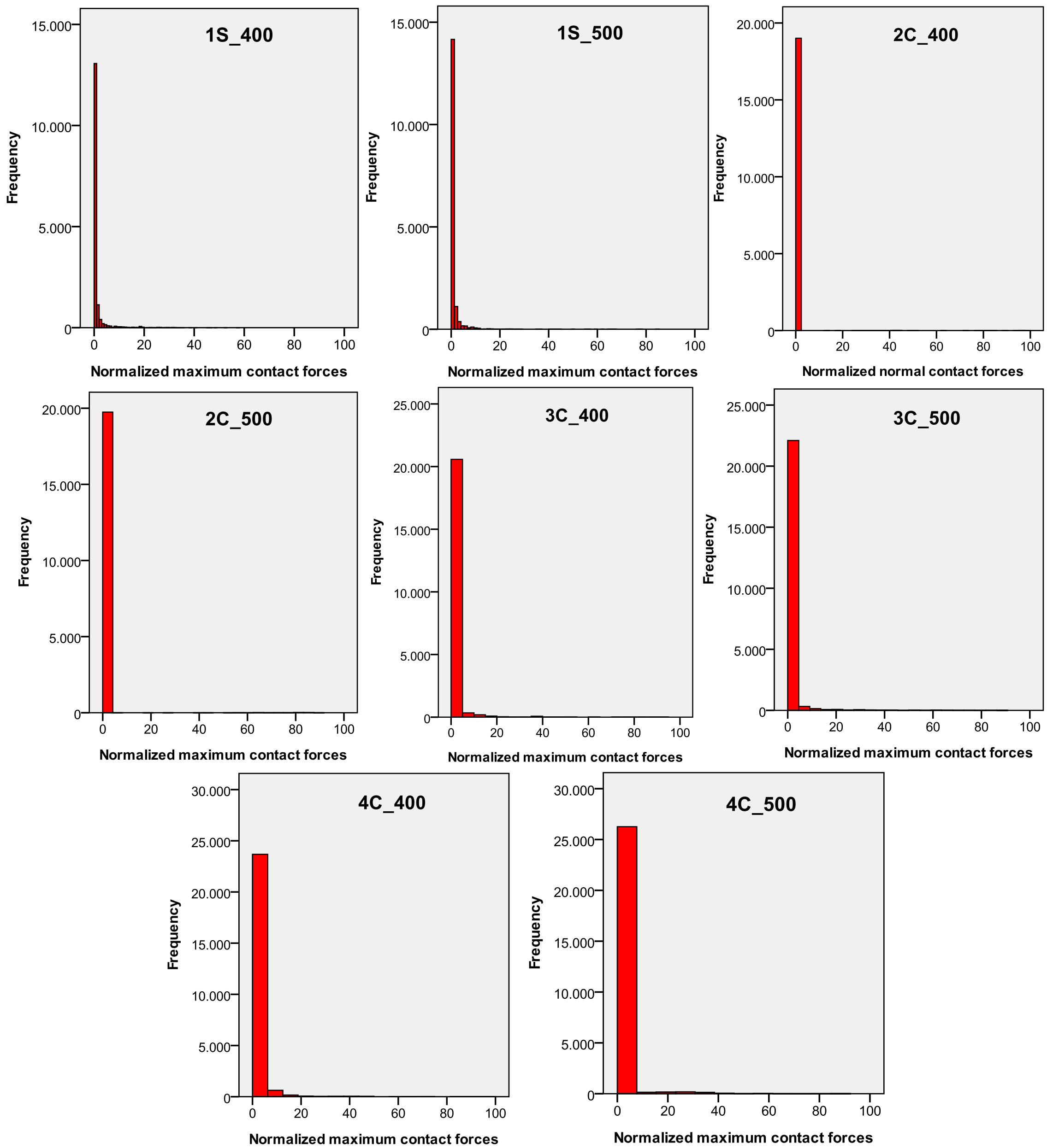


Fig. 6. statistical distribution of normalized contact forces, histograms

Table 9. 95th percentile of the modelled test

Confining pressure [kPa]	1S	2C	3C	4C
400	4.09	3.25	3.15	2.14
500	4.23	3.70	2.88	2.07

Finally the probability density function (PDF) that best fits the normalized normal contact forces distribution has been obtained. According to Marketos et al. (2007) [16], it was found that it has the following form:

$$g(f) = (f + a)^b \cdot e^{(c \cdot f + d)} \tag{1}$$

where f is the maximum normal contact force normalized by dividing it by the mean normal contact force at that loading level and a, b, c, d are coefficients of the model.

Table 10 summarizes, for all cases, the PDF coefficients and the R-squared values. Since they are very high, the PDF fit the data very well. The PDF coefficients, instead, are different among the mixtures examined and they did not follow a particular trend.

Table 10. Fitting constants

Type of mixture	a	b	c	d	R^2
1S	1	0.443	-0.306	-0.524	0.916
2C	1	0.104	-0.011	-0.136	0.947
3C	1	0.159	-0.020	-0.06	0.985
4C	1	0.094	-0.006	0.6	0.991

Figure 7 represents the PDF for the mixture 1S. For each type of grain, the PDF shows an exponential tail at large forces, a plateau near the mean force and a slight increase when the force towards zero.

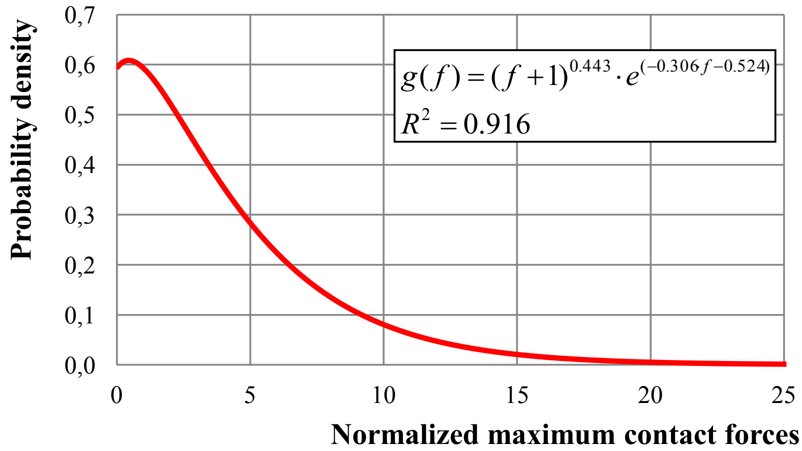


Fig. 7. PDF for mixture 1S

5. Conclusions

Based upon the developed research work, the following concluding remarks can be made:

- the degree of contact and interlocking of aggregates were found to be a function of the shape and angularity of the grains. Adding more angular particles to the assembly means achieving more aggregate contacts and a more uniform distribution of internal forces, with a better interconnection between elements and a significant improvement to the stability and the load distribution capability of the structure as well as to resistance to permanent deformation;

- the distribution of normalized normal contact forces has been computed and it shows exponential-like decay at large forces, a plateau near the mean force and a slight increase when the force towards zero;
- the DEM method was found to be a very useful tool to capture the effect that particle shape and angularity have on the performance of a granular mix for asphalt. So it represents an attractive alternative for use in predicting key physical properties of bituminous materials;
- on a micro-scale, using the DEM method, a "virtual laboratory" could be created to study the details of granular mechanics that cannot be measured in conventional laboratory tests. With the advancement in computer speed and storage capacity, this approach could provide a precise control of every variable being studied. Once the model is calibrated, it could be used to run as many simulations as required. The virtual testing environment would be an inexpensive tool to evaluate how changing different material and design factors can influence the mixture's response, reducing the number of physical laboratory tests required;
- the angular grains, modelled by clumps, still differ from real aggregates in asphalt mixtures. To overcame this problem, is found to be very helpful the combination of DEM and X-ray computed tomography technology, which obtained through rigorous image analysis the exact locations of aggregates and air voids of a real granular mix for asphalt. In this way DEM specimens will replicate the real materials very well.

References

[1] Campen, W. H., & Smith, J. R. (1948). A study of the role of angular aggregate in the development of stability in bituminous mixtures. Association of Asphalt Paving Technologists Proceedings, 17, 114-143.

[2] Ishai, I., & Gellber, H. (1982). Effect of geometric irregularity of aggregates on the properties and behavior of asphalt concrete. Association of Asphalt Paving Technologists Proceedings, 51, 494-521.

[3] Sanders, C.A., & Dukatz, E.L. (1992). Evaluation of percent fracture of hot-mixture asphalt gravels in Indiana. Effect of Aggregate and Mineral Filler on Asphalt Mixture Performance, Meininger R.C. editor.

[4] Kandhal, P. S., & Parker, F. Jr. (1998). Aggregate tests related to asphalt concrete performance in pavements. National Cooperative Highway Research Program Report 405, Transportation Research Board.

[5] Cheung, L.W., & Dawson, A.R. (2002). Effects of particle and mixture characteristics on performance of some granular materials. Transportation Research Record, 1787, 90-98.

[6] Shen, S., & Yu, H. (2011). Characterize packing of aggregate particles for paving materials: particle size impact. Construction and Building Materials, 25, 1362-1368.

[7] Cundall, PA., & Stark, O. (1979). A discrete numerical model for granular assemblies. Geotechnique, 1, 47-65.

[8] Buttlar, WG., & You, Z. (2001). Discrete element modeling of asphalt concrete: microfabric approach. Transportation Research Record, 1757, 111–118.

[9] Dondi, G., Bragaglia, M., & Vignali, V. (2007). Flexible pavement simulation with distinct particle element method. Proceedings of the 4th International SIIV Congress, Palermo, Italy.

[10] Mahmoud, E., Masad, E., & Nazarian, S. (2010). Discrete element analysis of the influences of aggregate properties and internal structure on fracture in asphalt mixtures. Journal of Materials in Civil Engineering, 22.

[11] PFC 3D manual. Version 4.0. Itasca Consulting Group Inc. Minneapolis.

[12] Dondi, G., Simone, A., Vignali, V., & Manganelli, G. (2012). Discrete particle element analysis of aggregate interaction in granular mixes for asphalt: combined DEM and experimental study. Proceedings of the 7th RILEM International Conference on Cracking in Pavements, 389-398, Delft, The Netherlands.

[13] Dondi, G., Simone, A., Vignali, V., & Manganelli, G. (2012). Numerical and experimental study of granular mixes for asphalts. Powder Technology, 232, pp. 31–40.

[14] O'Sullivan, C., Bray, JD., & Riemer, MF. (2004). Examination of the response of regularly packed specimens of spherical particles using physical tests and discrete element simulations. Journal of Engineering Mechanics, 10, 1140-1150.

[15] Cocurullo A., Airey G.D., Collop A.C., Sangiorgi C. (2008). Indirect Tensile versus Two Point Bending Fatigue Testing. ICE Transport, 161, pp. 207-220.

[16] Marketos, G., & Bolton, M.D. (2007). Quantifying the extent of crushing in granular materials: a probability-based predictive method. Journal of Mechanics and Physics of Solids, 55, 2142-2156.